# PYROLYSIS MODELING AND NUMERICAL SIMULATION OF RAIL CARRIAGE FIRE SCENARIOS FOR THE SAFE DESIGN OF A PASSENGER

# PYROLYSIS MODELING AND NUMERICAL SIMULATION OF RAIL CARRIAGE FIRE SCENARIOS FOR THE SAFE DESIGN OF A PASSENGER TRAIN

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## Abstract
The modeling of solid material pyrolysis is a critical issue for a reliable estimate of rail infrastructure fire resistance and the development of new firefighting systems. In this work a reliable procedure for the evaluation of the pyrolysis parameters required by FDS5 starting from cone calorimeter experimental data has been selected and tested. The results are encouraging as the cone calorimeter experiments have been successfully replicated by the CFD. The material pyrolysis properties derived from cone calorimeter tests have been used in the simulation of a rail carriage fire scenario. The behaviour of the fire scenario at different ignition source heat release rates has been analysed. Hot combustion products collected near the ceiling have been identified as one of the main causes of flashover. Therefore a system able to remove, or to cool, hot gases at the top of the carriage, which activates when a fire is detected, is expected to improve the performance of conventional firefighting systems.

## Introduction
In order to respect the recent regulations concerning safety in railway tunnels (DM 28/10/2005), Italian railway industries have to carefully review the performance of rail vehicles in terms of fire safety. In particular it is fundamental to develop and install proper firefighting systems to protect engine compartments, passenger carriages, night and restaurant coaches and all power electronic components installed in the train. As a consequence rail industries need proper tools to study fire propagation and efficiency of firefighting systems. In this field, the Computational Fluid Dynamics (CFD) can certainly give a great help to rail engineers in both understanding fire dynamics and choosing the best configuration of firefighting systems.

In this work the Fire Dynamics Simulator (FDS) code has been considered. It is a CFD code, developed by the National Institute of Standard and Technology (NIST), specifically devoted to the analysis of low velocity flows characterized by not negligible natural convection and buoyancy effects [1]. The code allows design engineers to easily perform numerical simulations of fire scenarios: different materials and geometries can be tested in reasonable time and with low cost in comparison with experimental full-scale tests. In FDS the turbulence is modeled using the Large Eddy Simulation (LES) approach with Smagorinsky sub-grid scale model; meshes can be classified as Cartesian structured grids.

The behavior of a train fire scenario is mainly determined by the pyrolysis of solid materials, together with ignition source characteristics. As a consequence, in order to perform a reliable simulation of a fire scenario, it is indispensable to accurately model the pyrolysis process. Pyrolysis can be defined as a "chemical decomposition of a material into one or more other substances due to heat alone" and "all solid combustibles must undergo pyrolysis in order to generate gaseous fuel vapors for flaming combustion" [2]. The energy required to convert a solid material into a vapor through pyrolysis will be referred to as "heat of vaporization" $\Delta H_v$. The pyrolysis process can follow different paths, depending on the characteristics of solid materials. For example cellulosic materials decompose directly to gaseous vapors whilst thermoplastics (such as polypropylene) follow a two step process (first of all a liquid is formed and then the liquid turns into a gaseous fuel) [2].

Despite its physical and chemical complexity, in FDS the pyrolysis process is simply modeled using an Arrhenius equation approach. In particular, in the Version 4 of FDS (FDS4) the mass flow rate (per unit area) of gaseous fuel generated by a given material is computed as[3]:

$$\dot{m} = \rho A e^{-E/(RT)} \tag{1}$$

where $A$ is the pre-exponential factor and $E$ is the activation energy. Thus the pyrolysis process is completely described when these two constants are given together with the heat of vaporization. Since these parameters are not usually available, the code also allows the user to specify other inputs which can be directly obtained in typical experimental tests. In FDS4 pyrolysis can be modeled by giving a critical mass flux and an ignition temperature (starting from these values the code internally compute the two Arrhenius constants) which can be derived from the cone calorimeter experimental test [3].

The Version 5 of the code (FDS5) offers several advantages in comparison with FDS4. It is possible to model multilayer materials and multistep pyrolysis reactions; water and residue can be easily added to the pyrolysis reaction products and the modeling of water-mist devices is simpler. In FDS5, pyrolysis of a given material is modeled using a more complex relation which considers multiple reactions and the amount of material produced as a residue of other reactions [4]. Considering a single-step pyrolysis reaction, in the case that no contribution is given by residues of other reactions, the FDS5 pyrolysis model can be rearranged as:

$$\frac{\partial Y}{\partial t} = -A'Y^n e^{-E'/(RT)} \tag{2}$$

where $Y$ is the normalized mass and $n$ is the reaction order. Once again, in order to model the pyrolysis process, the two Arrhenius constants $A'$ and $E'$ are required. Alternative inputs can also be assigned: they are called "reference temperature" and "reference rate" and they can be obtained using a thermo gravimetric experimental test [4] whilst no post-processing procedure was found in literature to directly derive these parameters from cone calorimeter experimental data.

The cone calorimeter test (ISO 5660) is the most commonly used tool to determine the pyrolysis properties and such measurements are the typical experimental data available in industrial material databases. Thus, in order to perform a fire scenario simulation using the FDS5 code, it is very interesting to develop a post-processing procedure able to derive FDS5 inputs from cone calorimeter experimental data so that such measurements can be used to set material properties in the new versions of FDS. In this paper a possible approach is described and validated using cone calorimeter data furnished by Trenitalia. The obtained pyrolysis parameters have been applied to the simulation of a rail carriage fire scenario: the influence of the ignition source thermal attach has been numerically investigated.

**Heat release rate**

The flammability hazard of a given material and the global evolution of a fire scenario is often represented in terms of Heat Release Rate (HRR) or Heat Release Rate Per Unit Area (HRRPUA) which is a measure of the rate at which a burning item releases chemical energy per unit exposed surface area of a burning material or specimen [2]. In a cone calorimeter test the heat release rate can be determined from measurements of the composition of product gases collected in an exhaust hood, usually using the oxygen consumption method. The heat release rate per unit area is equal to the product between mass loss rate per unit area and the effective heat of combustion $\Delta H_{c,eff}$. Since the mass loss rate is inversely proportional to the heat of vaporization, it is possible to write:

$$HRRPUA = \dot{m}\Delta H_{c,eff} = \frac{\Delta H_{c,eff}}{\Delta H_v} Q \tag{3}$$

where $Q$ is the material net absorbed heat flux. As shown in Equation (3), besides the net absorbed heat flux, the main parameter that controls the heat release rate is the ratio between the effective heat of combustion and the heat of vaporization. This ratio, also known as Heat Release Parameter (HRP), can be used to evaluate the flammability hazard of a material: hazardous materials usually have an HRP greater than 10 [2].

**Post processing of Cone Calorimeter data**

As said above, a procedure to directly derive FDS5 pyrolysis parameters from cone calorimeter tests was not found in literature. However a post-processing procedure to derive FDS4 pyrolysis parameters is available [5,6,7,8]. The procedure, based on thermal balances and experimental data correlations, was applied to six different materials. The selected materials are the ones that are expected to mainly influence the behavior of a passenger carriage fire scenario. Experiments were performed at three different exposure heat fluxes, replicating tests at each exposure heat flux in order to have a statistically representative set of data. Figure 1 shows the facility used in experimental tests whilst in Table 1 the pyrolysis parameters obtained in the post-processing are reported. It is important to note that ignition temperatures, one of the main outputs of the post-processing, are in agreement with data published in [9]; furthermore, the values of HRP indicate that all the materials have a low flammability hazard and this is mainly due to the presence of fire retardant additives.

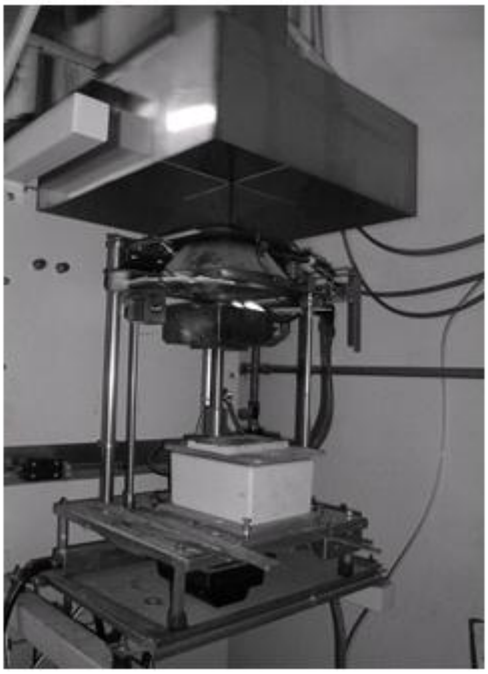

**Figure 1.** Cone calorimeter experimental facility.

| Parameter | **Seat** (cover + foam) | **Floor** (rubber) | **Curtain** | **Headrest** (cover) | **Wall** | **Ceiling** |
|---|---|---|---|---|---|---|
| Eff. heat of comb. [kJ/kg] | 23633 | 18480 | 15510 | 13093 | 14640 | 20950 |
| Heat of vaporization [kJ/kg] | 6478 | 5000 | 10782 | 4348 | 5572 | 11463 |
| Density [kg/m$^3$] | 95 | 1650 | 290 | 339 | 1652 | 867 |
| Ignition temperature [°C] | 352 | 419 | 436 | 398 | 427 | 462 |
| Heat capacity [kJ/(kg K)] | 0.345 | 1.92 | 8.33 | 8.32 | 1.26 | 1.24 |
| Mass loss rate peak [g/s] | 0.21 | 0.18 | 0.23 | 0.28 | 0.33 | 0.21 |
| HRP [-] | 3.65 | 3.77 | 1.44 | 3.01 | 2.63 | 1.83 |

**Table 1.** FDS4 pyrolysis parameters derived from cone calorimeter test.

In order to assess the reliability of the post-processing procedure, the cone calorimeter test was numerically replicated in FDS4 (Figure 2 shows the FDS model of the cone calorimeter) assigning the input parameters obtained in the post-processing. Numerical HRRPUA were compared with experimental measurements. Such a comparison showed the low reliability of the post-processing procedure (it might be due to the presence of fire retardant additives into the analyzed materials as also observed in [5]) and consequently the need of a further post-processing step in such a way as to obtain a much closer agreement with experimental data.

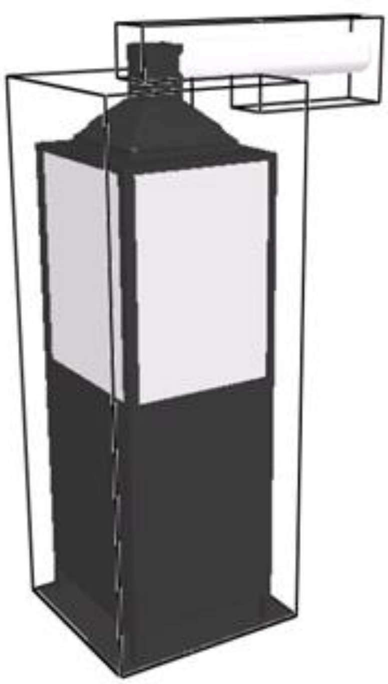

**Figure 2.** Cone calorimeter FDS model.

The adopted procedure is deeply described in [10]. In practice, the numerical simulation of the cone calorimeter test was performed again varying iteratively the main parameters affecting the HRRPUA until a good agreement with experiments was obtained. Figure 3 shows comparisons between numerical and experimental data. The dashed lines, labeled as "1$^{st}$ iteration", represent the heat release rate per unit area obtained using the parameters computed by means of the literature post-processing procedure: except for the seat and the floor a great disagreement between experimental and numerical data is evident. Final results obtained at the end of the iterative procedure are also reported: a good agreement with experiments was achieved for all materials using a heat of vaporization equal to a half of the original value.

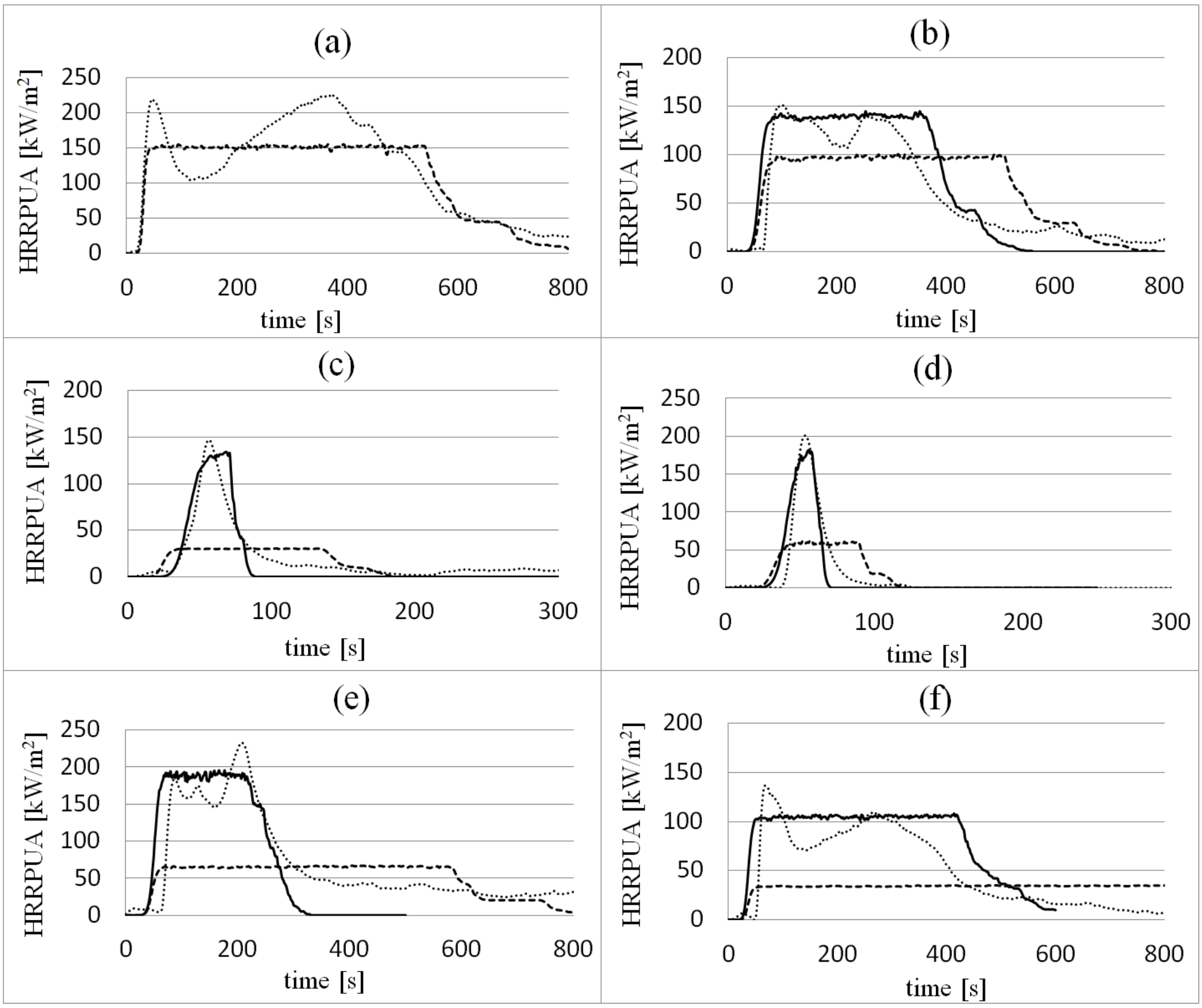


**Figure 3.** Comparison between experimental data and numerical results of FDS4 cone calorimeter simulations at Exposure Heat Flux = 50 kW/m$^2$: (........) Experiments, (- - - -) 1$^{st}$ iteration, (——) Final result [10]. (a) Seat, (b) Floor, (c) Curtain, (d) Headrest, (e) Wall, (f) Ceiling.

As stated before, once ignition temperature and critical mass flux are given, FDS4 internally computes the Arrhenius constants (see Equation (1)). Pyrolysis can be modeled in FDS5 by directly assigning the values of *A'* and *E'*. Although the FDS5 pyrolysis model is slightly different from the one implemented in FDS4, the Arrhenius constants extracted from FDS4 simulations can be a good starting point for a trial and error procedure based on FDS5 numerical simulations of the cone calorimeter test. It is important to note that the two pre-exponential factors *A* and *A'* have not the same units of measurement, so a more consistent value of *A'* can be computed as the ratio between *A* and a reference length. Numerical simulations of the cone calorimeter test have been performed again in the FDS5 framework; the values of *A'* and *E'* have been iteratively changed until a good agreement with experiments was achieved (see Figure 4).

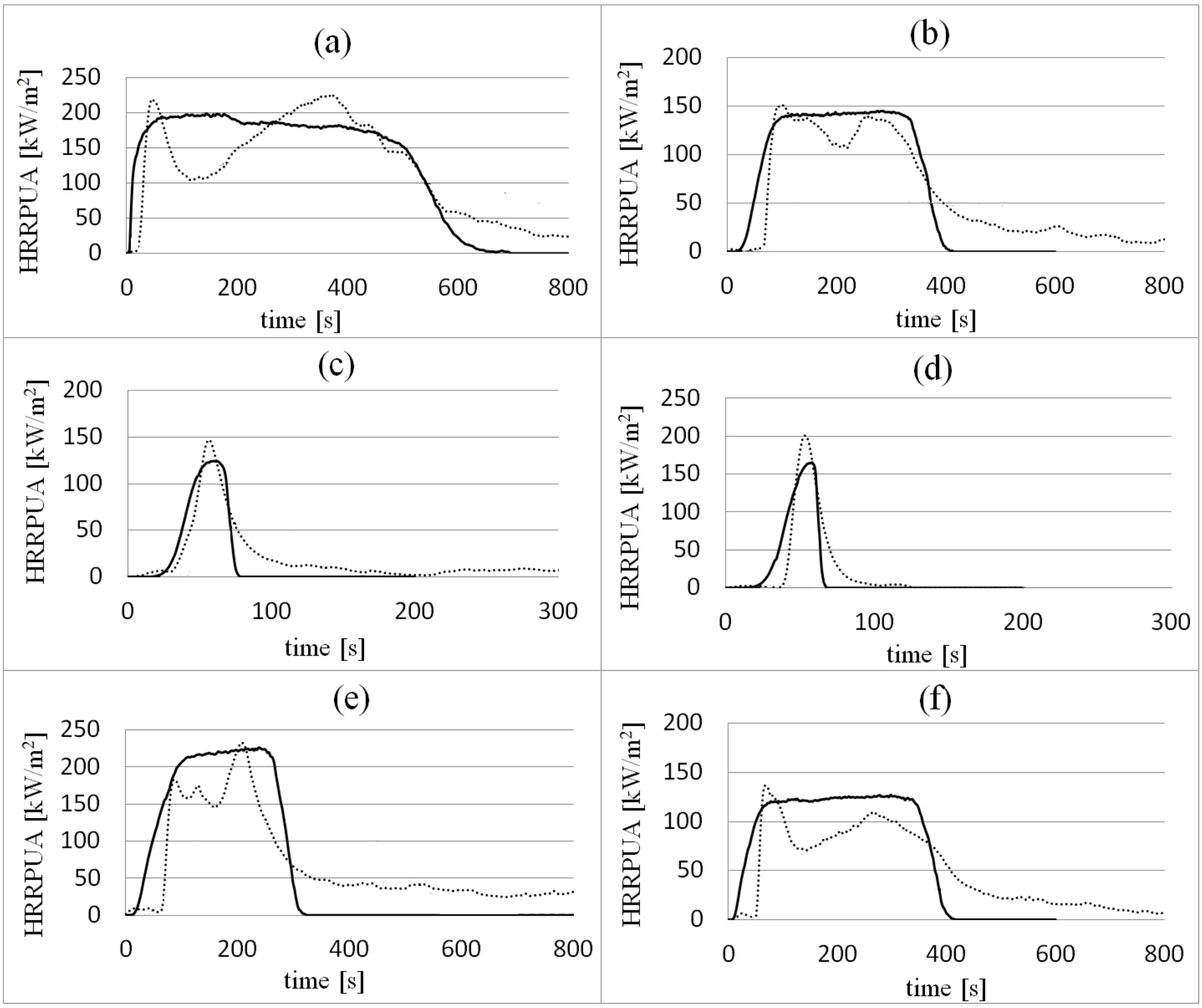


**Figure 4.** Comparison between experimental data and numerical results of FDS5 cone calorimeter simulations at Exposure Heat Flux = 50 kW/m$^2$: (**........**) Experiments, (**_____**) Final result. (a) Seat, (b) Floor, (c) Curtain, (d) Headrest, (e) Wall, (f) Ceiling.

**Numerical simulation of a passenger rail carriage**

Pyrolysis parameters obtained in the post-processing have been used to simulate a rail carriage fire scenario. The computational domain consists in a box with dimensions 26.0x3.5x3.5 m containing the carriage. Both the right and the left side of the carriage are open. The ignition source, a rectangular sheet vertically oriented, is placed on the left corner of the first seat (see Figure 5(a)). Figure 5(b) shows the particular heat release rate profile used to model the ignition source in all present simulations. In the first part of the simulation, the source heat release rate is held at the maximum value, then it gradually decays to zero.

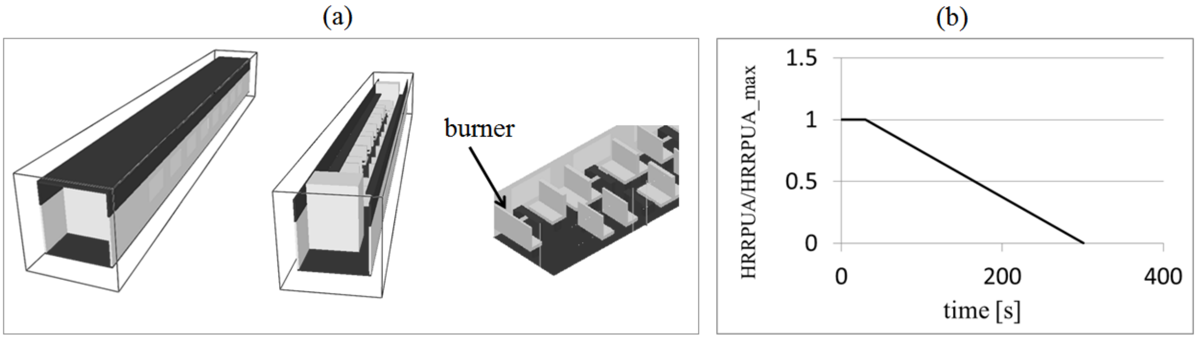


**Figure 5.** (a) Rail carriage fire scenario, (b) Heat release profile of the burner.

First of all a mesh sensitivity analysis was performed in order to find the best grid spacing able to guarantee a sufficient mesh independency. Figure 6 compares the HRR of two simulation characterized by the same fire scenario (i.e. the same geometry configuration and ignition source) but different grid refinement. The HRR curve obtained with the coarse mesh, dashed line, is sufficiently close to the one predicted with the finer mesh. Thus the coarse mesh has been employed in all the subsequent simulations resulting in a not negligible time saving.

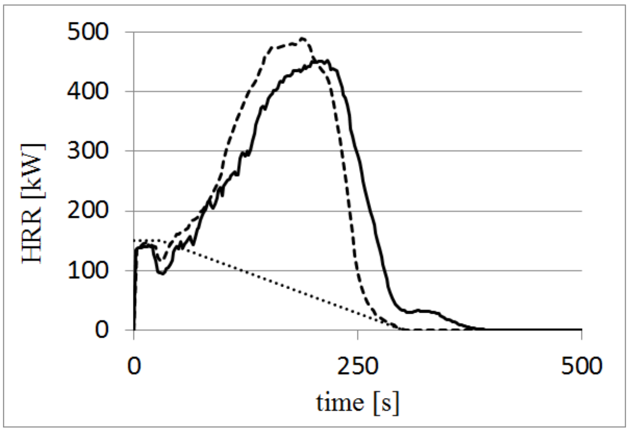


**Figure 6.** Mesh sensitivity analysis - ignition source maximum HRRPUA = 1500 kW/m$^2$; (........) Ignition source , (----)Total HRR-mesh 216x25x27, (——)Total HRR-mesh 320x35x38.

The behavior of the fire scenario at different source powers has been investigated. Table 2 illustrates the characteristics of the ignition source in the different cases that were considered. The equivalent gasoline mass, that is the mass of gasoline that generates the same amount of energy when completely burned, is also reported in order to give a more direct estimate of the ignition source potential.

| Source characteristic | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 |
|---|---|---|---|---|---|
| Surface area [m$^2$] | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| Total time [s] | 300 | 300 | 300 | 300 | 600 |
| Maximum power time [s] | 30 | 30 | 30 | 30 | 300 |
| Maximum HRRPUA [kW/m$^2$] | 1000 | 1500 | 2000 | 2500 | 5000 |
| Released energy [kJ] | 16525 | 24787 | 33050 | 41312.5 | 225125 |
| Equivalent gasoline mass [kg] | 0.39 | 0.59 | 0.79 | 0.98 | 5.36 |

**Table 2.** Ignition source characteristics.

Figure 7 to Figure 10 show the total HRR curve and the ignition source HRR curve of each case. The Total HRR curve represents the sum of the HRR of all the components of the fire scenario, including the burner. Furthermore, in Figure 11 to Figure 14 the temperature field in a cross section cutting the ignition source is reported. Temperature fields are very interesting since they give a great help in the understanding of fire propagation. In Case 1 and Case 2 only the first seat, where the ignition source is placed, burns. The burning occurrence is clearly indicated by the Total HRR curves that deviate from the ignition source HRR (see Figure 7). Case 3 is the limiting case between fire extinction and flashover. Hot gases generated by the burning seats on the left concentrate near the ceiling and move to the right until the blockage representing the toilet is reached. Because of the heat released by combustion products, the temperature of solid surfaces on the right rises up and when the material ignition temperature is exceeded burn occurs. The time sequence is shown in Figure 12. Two different flame fronts are generated, one on the left and one on the right, leading to the complete combustion of all combustible materials. Case 4 and 5 are two examples of flashover. Fire rapidly propagates to the entire carriage following the same mechanism described for Case 3: two different flame fronts form and meet near the center of the carriage (see Figure 13 and Figure 14).

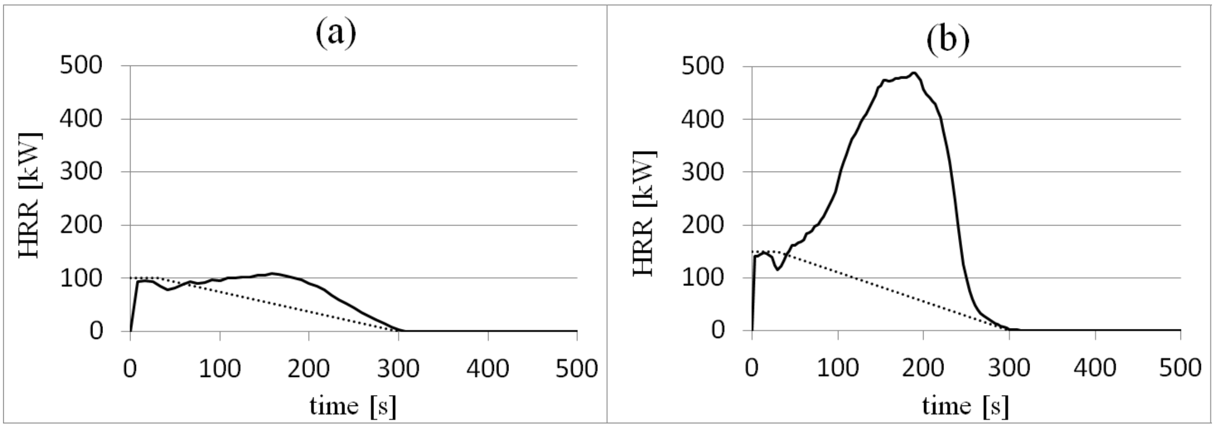


**Figure 7.** Rail carriage fire scenario HRR curves: (**........**) Ignition source, (**_____**) Total HRR; (a) Case 1, (b) Case 2.

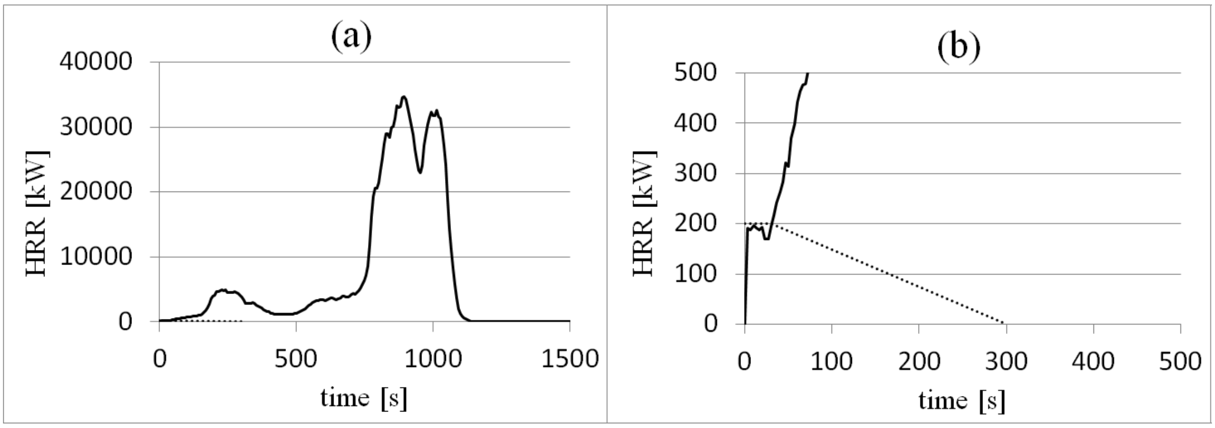


**Figure 8.** Rail carriage fire scenario HRR curves; Case 3: (**........**) Ignition source, (**_____**) Total HRR; (a) Overview, (b) Detail.

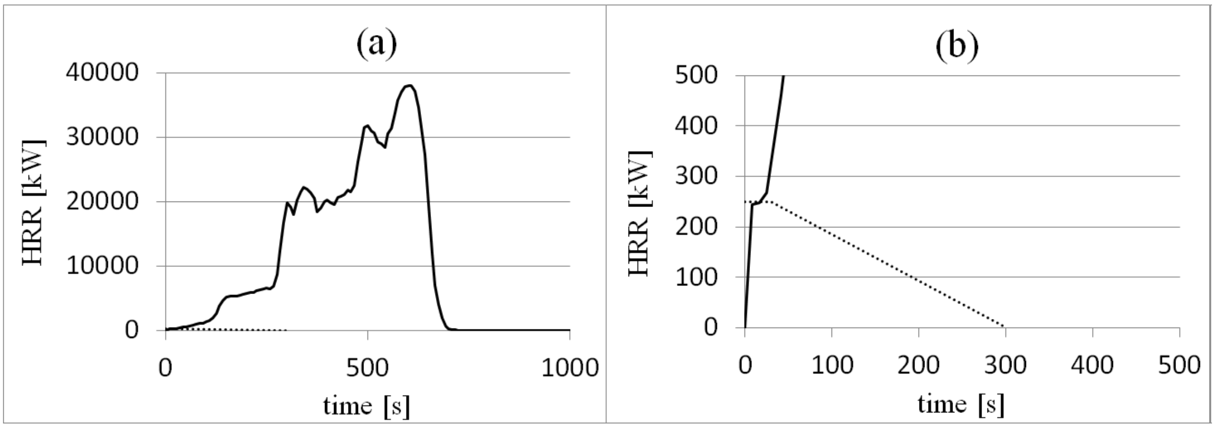


**Figure 9.** Rail carriage fire scenario HRR curves; Case 4: (........) Ignition source, (_____) Total HRR; (a) Overview, (b) Detail.

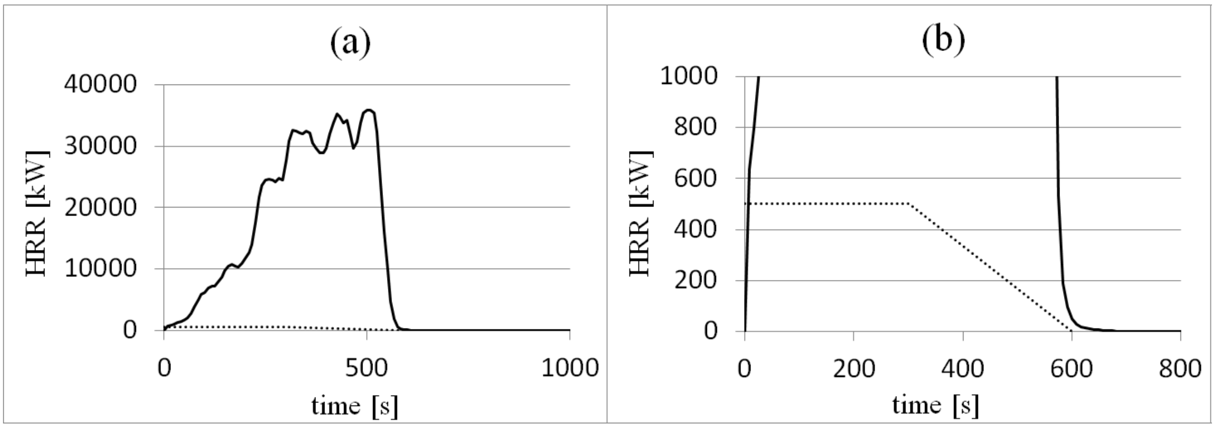


**Figure 10.** Rail carriage fire scenario HRR curves; Case 5: (........) Ignition source, (_____) Total HRR; (a) Overview, (b) Detail.

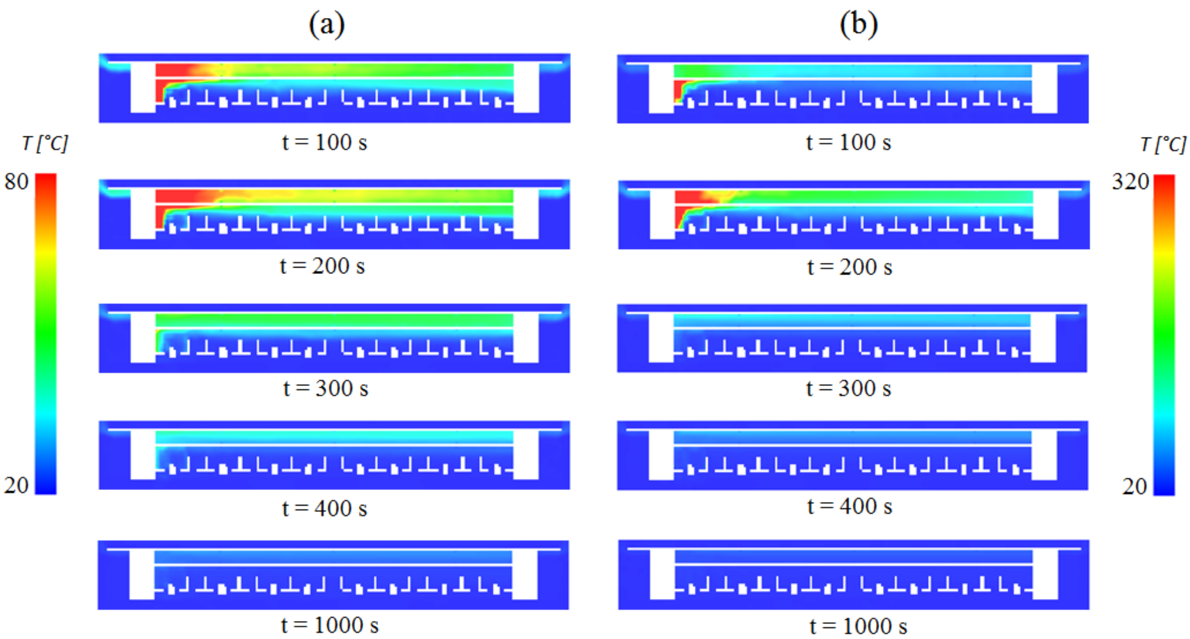


**Figure 11.** Temperature field time history in a cross section cutting the burner: (a) Case 1, (b) Case 2.

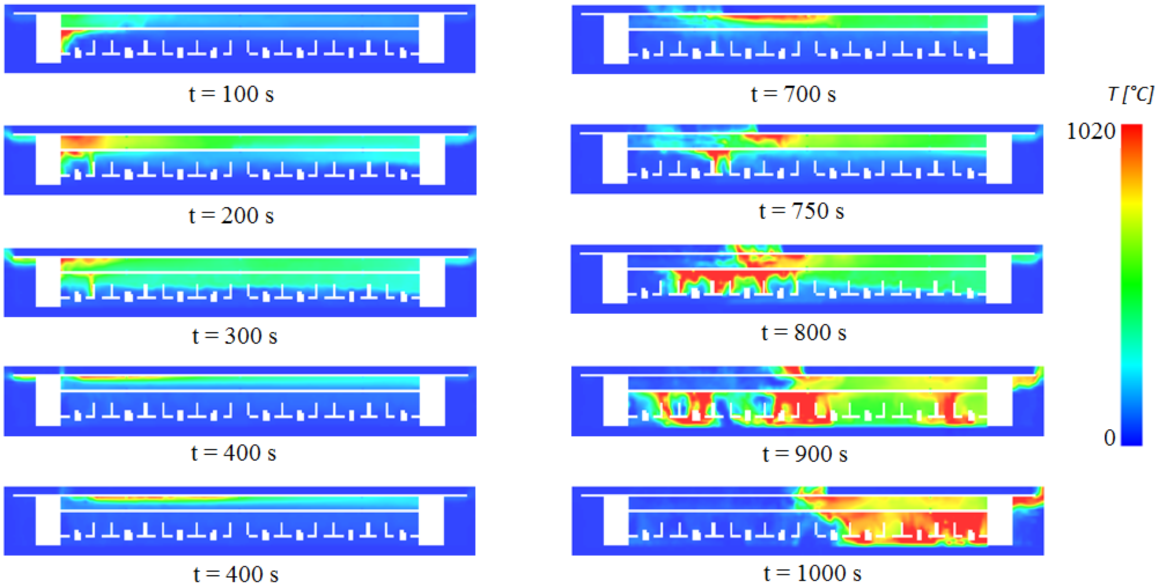


**Figure 12.** Temperature field time history in a cross section cutting the burner: Case 3.

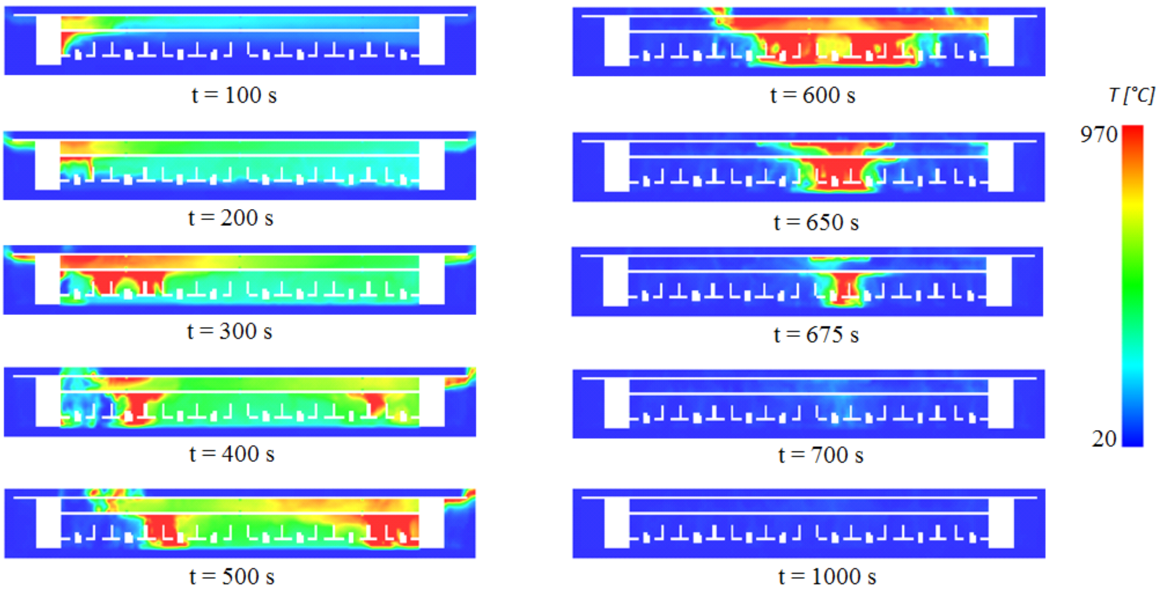


**Figure 13.** Temperature field time history in a cross section cutting the burner: Case 4.

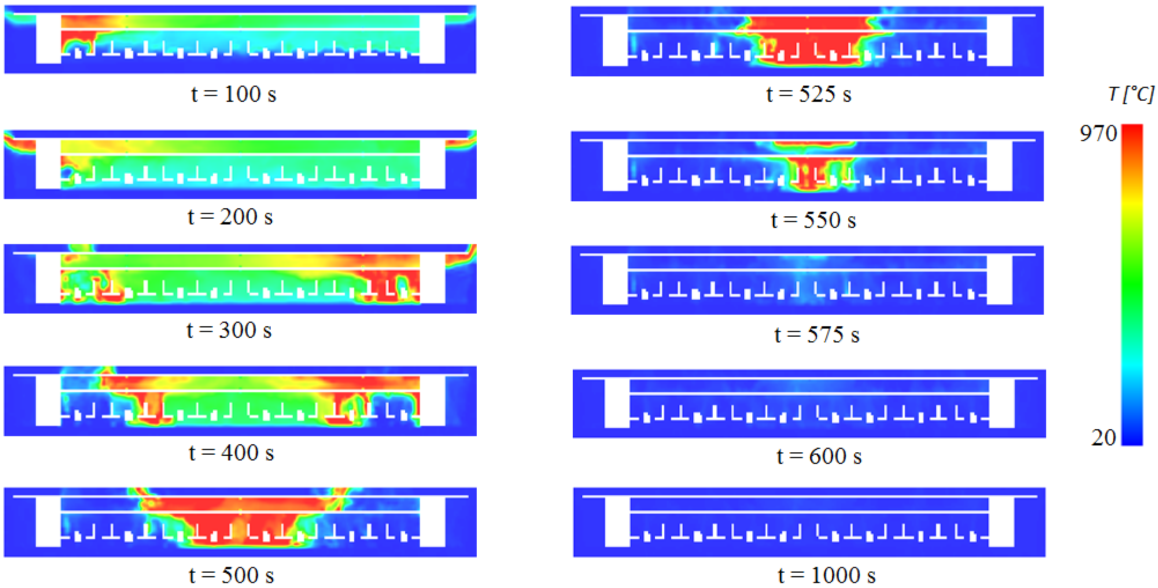

**Figure 14.** Temperature field time history in a cross section cutting the burner: Case 5.

## Conclusions

In this work a reliable procedure for the evaluation of the pyrolysis parameters required by FDS5 starting from cone calorimeter experimental data has been selected and tested. Six different materials, the most important in a typical passenger carriage fire scenario, have been analysed. The results are encouraging as the cone calorimeter experiments have been successfully replicated by the CFD.

Material properties derived from cone calorimeter tests have been used in the simulation of a rail carriage fire scenario. Numerical results showed that one of the main causes of flashover is related to the hot combustion products collected near the ceiling. Therefore a system able to remove, or to cool, hot gases at the top of the carriage, which activates when a fire is detected, is expected to improve the performance of conventional firefighting systems.

Future works will be focused on selecting and testing firefighting systems. Furthermore, a full scale experimental test of a rail carriage fire scenario has also been planned in order to assess the reliability of FDS5 simulations.

## Acknowledgements

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## Nomenclature

| | | |
|---|---|---|
| *A* | Pre-exponential factor (FDS4) | [m/s] |
| *A'* | Pre-exponential factor (FDS5) | [1/s] |
| *E* | Activation energy (FDS4) | [kJ/kmol] |
| *E'* | Activation energy (FDS4) | [kJ/kmol] |
| *HRP* | Heat Release Parameter | [-] |
| *HRR* | Heat Release Rate | [kW] |
| *HRRPUA* | Heat Release Rate Per Unit Area | [$kW/m^2$] |
| $\dot{m}$ | Mass loss rate | [$kg/(s\ m^2)$] |
| *n* | Reaction order | [-] |
| *Q* | Net absorbed heat flux | [$kW/m^2$] |
| *t* | Time | [s] |

| | | |
|---|---|---|
| $T$ | Temperature | [K] |
| $Y$ | Normalized mass | [-] |
| $\rho$ | Density | [kg/m$^3$] |
| $\Delta H_{c,eff}$ | Effective heat of combustion | [kJ/kg] |
| $\Delta H_v$ | Heat of vaporization | [kJ/kg] |

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